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Electronic Structure and Superconductivity in $Na_xCoO_2 \cdot yH_2O$

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Introduction: The Navy has long had an interest in developing a superconducting homopolar motor for ship propulsion. A giant step toward practical implementation came with the discovery of high critical temperature, or high T_c, superconductors. These are compounds capable of carrying a resistanceless current at temperatures above that of liquid nitrogen. The performance of these motors depends sensitively on the ability to create and stabilize a large current density. Therefore, detailed understanding of the microstructure and underlying physics of superconducting materials is crucial to further technological development.

The experimental breakthrough of synthesizing high T_c compounds was accompanied by the realization that well-established theories explaining the microscopic origins of superconductivity could not adequately explain these new materials. The search for a coherent and complete description of unconventional superconductivity as a step toward development of even better devices and applications is therefore a primary concern of materials science theory.

Superconductivity is an intrinsically quantum mechanical phenomenon arising from pairing between electrons. Since each electron individually has its own quantum properties, the paired-state characteristics depend on the detailed properties of unpaired electrons in the normal (metallic) state. An instability of the Fermi surface(s) of this normal state causes condensation into a superconducting fluid of electron pairs. From an understanding of Fermi surface geometry, many properties of the superconducting state can be deduced.

$Na_xCoO_2 \cdot yH_2O$: The newly discovered[1] superconductor, $Na_xCoO_2 \cdot yH_2O$ (NCO) has a relatively low critical temperature (T_c = 4K), but it shares several important commonalities with traditional high T_c materials: it is a layered, transition metal compound (Fig. 4), its superconducting phase depends on electron doping, and a growing body of evidence indicates an unconventional pairing state. On the other hand, NCO is a Co-, rather than Cu-based compound, and the triangular arrangement of ions is different from the square plaquettes common to most high T_c structures. NCO therefore provides a unique opportunity to investigate how superconducting properties depend on the particularities of structure and chemistry.

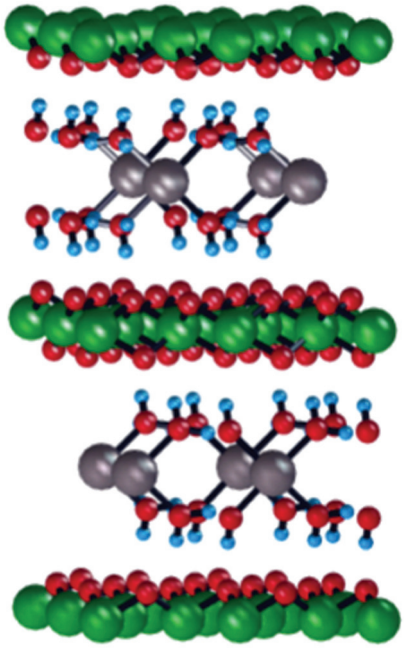

FIGURE 4
Crystal structure of $Na_xCoO_2 \cdot yH_2O$: green spheres denote Co, gray Na, red O, and blue H.

Computational Approach: Density functional theory (DFT) methods, developed by W. Kohn (for which he later won a Nobel prize) with ONR support, provides a state-of-the-art description of the quantum ground state of condensed matter systems. For the research reported here, we used several computational implementations of DFT, developed both inside our group (the NRL tight-binding method) and outside. This allowed high-precision computation of the electronic structure, Fermi surface geometry, and magnetic properties, all fundamental to understanding superconductivity.

Symmetry and Superconductivity: Our calculations show that the hexagonal, quasi-two-dimensional structure of NCO is reflected in the symmetry of its Fermi surfaces (Fig. 5). The six smaller cylindrical surfaces, when translated by a particular vector, can be made to lie directly atop one another, or "nest." This nesting gives rise to spin fluctuations with the wavelength of the nesting vector. We calculated the real and imaginary parts of the low-frequency susceptibility (Fig. 6) and found strong peaks, indicating the positions of nesting-driven spin fluctuations in reciprocal

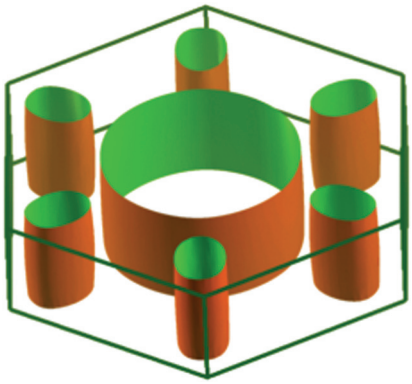

FIGURE 5
Calculated Fermi surface of $Na_xCoO_2 \cdot yH_2O$.

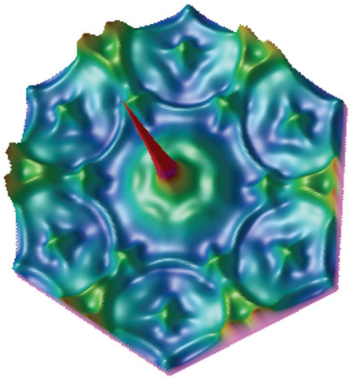

FIGURE 6
Calculated imaginary part of the magnetic susceptibility at low frequency as a function of the two-dimensional wave vector (in arbitrary units).

space. Depending on the symmetry properties of the superconducting state, these spin fluctuations can either be constructive or destructive to the formation of electron pairs. Our analysis shows[2] that spin fluctuations in NCO are destructive to all previously considered superconducting states. A superconducting state is generally characterized by a wave vector-dependent order parameter and a particular spin pairing. To be compatible with the calculated nesting properties, the superconducting state of NCO would need to be both triplet, meaning that both electron spins are aligned, and have spatial s-wave symmetry, implying a uniform order parameter. Such a superconducting state has been discussed before in connection with liquid helium but it has never been observed experimentally. Most interestingly, this state violates the Pauli exclusion principle for the electron pairs since the multiplication of the even (triplet) spin part with the even (s-wave) spatial part produces an overall wavefunction that does not satisfy the necessary condition of having odd parity. The Pauli principle is, however, restored by introducing an odd parity in the frequency part of the order parameter. The proposed state, although extremely unusual, not only follows from our calculations but is also compatible with all currently reported experimental evidence.

Summary: Computational investigation of superconducting compounds provides insight into how experimentally tunable parameters, such as doping or pressure, affect the underlying mechanisms that give rise to superconductivity. Careful study of the electronic structure properties of NCO reveals the possibility of a truly unusual type of superconductivity, more unconventional yet than even the enigmatic high-temperature superconductors. A final understanding of unconventional superconductors could provide the basis for development of new, high critical temperature materials for which potential applications in both Naval and civilian technologies are nearly unlimited.

[Sponsored by ONR]

References

[1] K. Takada, H. Sakurai, E. Takayama-Muromachi, F. Izumi, R.A. Dilanian, and R. Sasaki, "Superconductivity in Two-dimensional CoO_2 Layers," *Nature* **422**, 53-55 (2003).

[2] M.D. Johannes, I.I. Mazin, D.J. Singh, and D.A. Papaconstantopoulos, "Nesting, Spin-fluctuations, and Odd-gap Superconductivity in $Na_xCoO_2 \cdot yH_2O$," *Phys. Rev. Lett.* **93**, 433-439 (2004).